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GALVANOMAGNETIC EFFECTS IN POLYCRYSTALLINE MANY VALLEY SEMICONDUCTORS

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SUMMARY

Formal transport theory is used to derive expressions for the isothermal conductivity, Hall conductivity, and magnetoconductivity of semiconductors with anisotropic multivalley band structure. The theory is applied to quasi isotropic polycrystalline materials and developed for arbitrary statistics and magnetic field strengths. An annotated bibliography is included.

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CONTENTS

Summary	i
Notation	v
INTRODUCTION	1
THEORY FOR A SINGLE VALLEY	2
The Model	2
Solution of the Transport Equation	2
Conductivity for a Single Valley	4
EXTENSION OF THE THEORY TO MANY VALLEYS	7
Theory for a Single Crystal	7
Theory for Polycrystalline Materials	4
CONCLUSION	.9
ANNOTATED BIBLIOGRAPHY 2	0
References	1

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Notation

Vectors of any dimension are boldface (a) in matrix notation and have a single subscript (a_i) in tensor notation. Second rank tensors (A_{ij}) are written as square matrices and appear in sans-serif typeface (A). A dot between two quantities written in matrix notation corresponds to contraction on one index in tensor notation. Where confusion may arise in transferring from one notation to another, a matrix in the form A is written in tensor notation as $(A)_{ij}$.

A list of symbols used in this report follows. The number refers to the equation (page) where the symbol first appears.

Α	coordinate transformation matrix	42
а	dimensionless function of $\boldsymbol{\varepsilon}_{\mathbf{k}}$ and \mathbf{H}	61
c	speed of light	3
c, c ₁ , c ₂	elements of isotropic fourth rank tensor	53
$\mathbf{r}_{_{\mathbf{i}}}$	integral over surface of constant $\tilde{\kappa}_{\mathbf{k}}$	14
D(H)	denominator of energy integral for large H	19
$\mathcal{E}_{\mathbf{k}}$	energy of electron with wave number k	1
e	absolute value of electronic charge	3
E	electric field strength	3
$\mathbf{F}^{(n)}$ ($\mathbf{\xi_k}$)	energy factor in transport integral	60
f, f _o	perturbed and equilibrium electron distribution functions	3
Н	magnetic field	3
ħ	Planck's constant $\div 2\pi$	1
I	electric current	49
ŧ	unit matrix	9
g(n)	transport integral for small H	17
J	current density	10
$\mathbf{k_i}$, \mathbf{k}	electron wave vector	1
K(u)(H)	transport integral for large H	22
l	relaxation time proportionality constant	2
m_{i}	component of effective mass tensor corresponding to direction $\mathbf{k}_{_{1}}$ in standard orientation	1
m	effective mass tensor	7
N	number of valleys in polycrystalline material	50
זוי	constant factor in transport integrals	17

\mathbf{s}	area vector of plane through a sample of polycrystalline material	49
\mathbf{s}_{i}	area vector of a single crystal sliced by plane S	49
$\mathbf{v}_{\mathbf{k}}$	velocity of electron with wave vector k	3
w	wave vector for spherically symmetric energy surfaces	page 5
x, x'	arbitrary vectors	25
x	= $\cos \theta$ (when not a cartesian coordinate)	61
α	relaxation time energy exponent	2
Δ	determinant of $m = m_1 m_2 m_3$	9
δ_{ij}	kronecker delta symbol	46
δ_{ijk}	permutation symbol	31
θ	Euler angle or polar angle, depending on context	42
Λ	anisotropy parameter	55
σ(H)	conductivity tensor	23
$\left\langle \sigma \left(H\right) \right\rangle$	conductivity tensor averaged over orientation	page 15
au	relaxation time	2
$\Phi(\mathbf{k})$	energy factor in deviation of distribution function from equilibrium	4
ϕ	Euler angle	42
ψ	Euler angle	42
Ω_{ijkl}	magnetoconductivity tensor for weak H	32
ω	energy dependent factor in D(H)	48

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INTRODUCTION

The *many valley* model of the energy band structure of semiconductors has proved to be a fruitful and illuminating concept in the explanation of electron transport phenomena. Recently it has been shown that in addition to germanium and silicon, for which the model was originally developed, a number of other semiconductors of current technical importance exhibit a many valley band structure.* Present treatments of the theory of transport phenomena for these substances are principally concerned with the results for single crystal specimens. Indeed, it was through the measurement of single crystal properties that the failure of the spherically symmetric theory first became evident. Nevertheless, it is of some interest to determine how the parameters characterizing the single crystal case reveal themselves in measurements on polycrystalline samples.

We would expect a sample to show isotropic symmetry, as in the spherically symmetric case, but in place of the conventional scalar effective mass we would expect to find combinations of the "longitudinal" and "transverse" effective masses which characterize a single valley. Just what combinations of these parameters appear and whether they appear in the same combinations in different transport phenomena are to be determined by direct appeal to the general theory.

What follows are a review of the mathematical techniques of the many valley theory and an analysis of the manner in which the theory yields results for polycrystalline materials. The first part is a review of the methods of solving the Boltzmann transport equation for a single valley. The second section is a detailed discussion of the mathematical problem of describing real materials in terms of the single valley parameters.

Most of this material may be found in the references. An attempt is made here to simplify the treatment and provide a straightforward and self-contained presentation of the theory of the isothermal galvanomagnetic effects for polycrystalline many valley semiconductors. The development for the case of strong magnetic fields has not been given elsewhere.

^{*}See discussion group sections of Reference 1, and references cited in Reference 2.

THEORY FOR A SINGLE VALLEY

The Model

The postulates for the simple many valley model were formulated in 1954 by Abeles and Meiboom and by Snibuya (References 3 and 4). In this model the surfaces of constant energy in crystal momentum space (k space) are assumed to be ellipsoids of the form

$$\mathcal{E}_{k} = \frac{\hbar^{2}}{2} \left(\frac{k_{1}^{2}}{m_{1}} + \frac{k_{2}^{2}}{m_{2}} + \frac{k_{3}^{2}}{m_{3}} \right) , \qquad (1)$$

where m_i is the component of the effective mass tensor in the direction of k_i . It is evident that one valley of this form will not in general possess the symmetry of the crystal. To achieve this symmetry a set of such valleys in the Brillouin zone must be postulated, arranged so that the sum of the properties of the minima will exhibit the symmetry of the crystal. In many cases several such sets may satisfy the symmetry requirements. Herring has pointed out that such surfaces may be complicated by degeneracy (Reference 5), but, since there are sufficient cases of interest in which it is not important, this complication will not be discussed here. Neither will the possibility of an anisotropic relaxation time be discussed. However the relaxation time will depend on an arbitrary power of energy δ_v . Thus

$$\tau(\mathcal{E}_{\mathbf{k}}) = t\mathcal{E}_{\mathbf{k}}^{\alpha} , \qquad (2)$$

where ℓ and a are independent of energy (but perhaps dependent on temperature). Finally, we shall ignore any contribution to τ arising from the scattering of electrons between different valleys (intervalley scattering) and focus attention on the processes taking place in a single valley (intravalley scattering). This simplification allows the representation of the properties of a real material as a sur over the properties of a single valley. For a discussion of the effect of these approximations on the final results, see the excellent articles by Herring (Reference 5) and Herring and Vogt (Reference 6).

Solution of the Transport Equation

This section will consider methods of solving the isothermal Boltzmann transport equation for the electron distribution function f:

$$\frac{-e}{\hbar} \left[\mathbf{E} + \frac{1}{c} \left(\mathbf{v}_{\mathbf{k}} \times \mathbf{H} \right) \right] + \nabla_{\mathbf{k}} \mathbf{f} + \frac{\mathbf{f} - \mathbf{f}_{0}}{\tau \left(\boldsymbol{\xi}_{\mathbf{k}} \right)} = 0 . \tag{3}$$

E and H are the electric and magnetic field strengths, \mathbf{v}_{k} is the velocity of an electron with energy \mathcal{E}_{k} , and - \mathbf{e} is the electronic charge. Following the conventional approach, let

$$\mathbf{f} = \mathbf{f}_0 - \mathbf{\phi}(\mathbf{k}) \frac{\partial \mathbf{f}_0}{\partial \mathcal{E}_{\mathbf{k}}}$$
, (4)

where f_0 is the Fermi-Dirac distribution function. Substitution of Equation 4 into Equation 3 yields

$$\Phi(\mathbf{k}) = \frac{-e\tau}{\hbar} \left[\hbar \mathbf{E} \cdot \mathbf{v_k} + \frac{1}{c} \mathbf{H} \cdot \mathbf{v_k} \times \nabla_{\mathbf{k}} \Phi(\mathbf{k}) \right] , \qquad (5)$$

where a term of the order $\mathbf{E}\cdot\nabla_{\mathbf{k}}\Phi(\mathbf{k})$ has been neglected and the relation $\nabla_{\mathbf{k}}\mathcal{E}_{\mathbf{k}}=\hbar \mathbf{v}_{\mathbf{k}}$ has been used to simplify the expression.

The form of Equation 5 suggests an iterative method of solution for small values of H. If the term in H is ignored, the "zeroth order" approximation is

$$\Phi^{(0)}(\mathbf{k}) = -e\tau \mathbf{E} \cdot \mathbf{v}_{\mathbf{k}}, \qquad (6)$$

which, substituted into Equation 5, gives

$$\Phi^{(1)}(\mathbf{k}) = \frac{-e\tau}{\hbar} \left(\hbar \mathbf{E} \cdot \mathbf{v}_{\mathbf{k}} - \frac{\hbar e\tau}{c} \mathbf{H} \cdot \mathbf{v}_{\mathbf{k}} \times \mathbf{m}^{-1} \cdot \mathbf{E} \right). \tag{7}$$

The relation $h^2 m^{-1} = \nabla_k \nabla_k \delta_k$ has been used; m^{-1} is the inverse effective mass tensor. In that which follows it will be assumed that, for the single valley under consideration, the coordinate axes in k space lie along the principal axes of the ellipsoid. This will be the *standard orientation*. Higher order approximations are obtained similarly. For example,

$$\Phi^{(2)}(\mathbf{k}) = \frac{-e\tau}{\hbar} \left[\hbar \mathbf{E} \cdot \mathbf{v}_{k} - \frac{\hbar e\tau}{c} \mathbf{H} \cdot \mathbf{v}_{k} \times \mathbf{m}^{-1} \cdot \mathbf{E} \right.$$

$$\left. + \frac{e^{2} \tau^{2}}{c^{2}} \mathbf{H} \cdot \mathbf{v}_{k} \times \nabla_{k} \left(\mathbf{H} \cdot \mathbf{v}_{k} \times \mathbf{m}^{-1} \cdot \mathbf{E} \right) \right]. \tag{8}$$

Higher approximations than this need not be computed if the magnetic field is sufficiently weak.

Although it is not obvious from Equations 6-8, the series solution given by this technique can be expressed in a closed form. Wilson shows for the isotropic case (m⁻¹ a scalar) how this form may be obtained by direct solution of Equation 5 (Reference 7, page 210). The procedure when m⁻¹ is a tensor is not significantly different and leads to the exact form:

$$\Phi(\mathbf{k}) = \frac{-\operatorname{e}_{\mathcal{T}} \mathbf{v}_{\mathbf{k}} \cdot \left[\mathbf{E} - \frac{\tau e}{c} \left(\mathbf{m}^{-1} \cdot \mathbf{E} \right)_{\times} \mathbf{H} + \left(\frac{\tau e}{c} \right)^{2} \frac{1}{\Delta} \mathbf{m} \cdot \mathbf{H} \left(\mathbf{E} \cdot \mathbf{H} \right) \right]}{1 + \left(\frac{\tau e}{c} \right)^{2} \frac{1}{\Delta} \mathbf{H} \cdot \mathbf{m} \cdot \mathbf{H}}, \tag{9}$$

where $\triangle = \det m$, and $m \cdot m^{-1} = m^{-1} \cdot m = 1$, the unit tensor. Equation 9 must be used to compute transport properties when strong magnetic fields are present. Unfortunately the appearance of m in the denominator of this form causes a vast complication. For this reason most discussions of the galvanomagnetic effects concentrate on Equation 8, which is only applicable in the limit of low fields.

Another method of solving Equation 5 has been employed by a number of workers.* This approach involves transforming to a coordinate system in which the three independent components of the effective mass tensor are equal. The transformed equation may then be solved as in the spherically symmetric case and the solution transformed back to the original anisotropic system. This procedure side-steps some computational work, but the results are the same as for the methods previously described. In the next section this transformation will be used to simplify the transport integrals.

An approach entirely different from that outlined here is discussed by McClure (Reference 9). Although his treatment is more general, it hardly lends itself to practical computations of the sort performed here.

Conductivity for a Single Valley

Now we shall consider in some detail the result of substituting the expression for $\Phi(k)$ from Equation 8 or 9 into the integral defining the electric current density J:

$$J = \frac{-e}{4\pi^3} \int v_k f d^3k$$

$$= \frac{e}{4\pi^3} \int_{\mathbf{V_k}} \Phi(\mathbf{k}) \frac{\partial f_0}{\partial \mathbf{E_k}} d^3k , \qquad (10)$$

where d³k denotes a volume element in crystal momentum space. The integration is to be taken over all space. Evidently this substitution will lead to quite different forms depending on whether Equation 8 or 9 is used, although for weak magnetic fields they should give the same results. Each form requires special treatment.

Case 1-Weak Magnetic Fields

By writing out Equation 8 in component form and simplifying, the entire expression becomes

$$\Phi^{(2)}(\mathbf{k}) = \frac{-e\tau}{\hbar} \left\{ \hbar \mathbf{E} \cdot \mathbf{v}_{\mathbf{k}} - \frac{\hbar e\tau}{c} \mathbf{v}_{\mathbf{k}} \cdot \left(\mathbf{m}^{-1} \cdot \mathbf{E} \right) \times \mathbf{H} + \left(\frac{e\tau}{c} \right)^{2} \frac{1}{\Delta} \mathbf{v}_{\mathbf{k}} \cdot \left[\left(\mathbf{m} \cdot \mathbf{H} \right) \mathbf{H} - \left(\mathbf{H} \cdot \mathbf{m} \cdot \mathbf{H} \right) + \right] \cdot \mathbf{E} \right\},$$
(11)

where $\triangle = m_1 m_2 m_3$ and I is the three-dimensional unit matrix.

^{*}References 2 and 6 are representative. Reference 8 also includes a discussion of this technique.

Substituting this into Equation 10 yields

$$J = -\frac{e^2}{4\pi^3} \int_{\mathbb{T}} v_k |v_k| + E \, \frac{\partial \, f_0}{\partial \xi_k} |d^3k| + \frac{e^3}{4\pi^3} \frac{e^3}{e} \int_{\mathbb{T}} ^2 |v_k| |v_k| + \left(H_{\mathbb{T}} |\mathsf{m}^{-1}| \right) | + E \, \frac{\partial \, f_0}{\partial \xi_k} |d^3k|$$

$$=\frac{e^4}{4\pi^3\,c^2}\,\frac{1}{\triangle}\int_{\mathbb{T}}^3\,v_k^{}\,v_k^{}+\left[\left({}_{\text{m}}\!+\!H\right)\,H+\left(H\!+\!m\!+\!H\right)\,I\right]+\,E\,\frac{\partial\,f_0}{\partial\mathcal{E}_k^{}}\,\,\mathrm{d}^3k\ . \tag{12}$$

Now recall that $\hbar k = m \cdot v_k$. Since the region of integration includes all directions and magnitudes of k, all integrals in Equation 12 containing a product $v_i \ v_j \ (i \neq j)$ will vanish. The remaining integrals each contain a factor $v_i^2 = \hbar^2 \ k_i^2 / m_i^2$ (i = 1, 2, 3). A further simplification results from the relation

$$d^{3}k = \frac{dS d\mathcal{E}_{k}}{\left| \bigvee_{k} \mathcal{E}_{k} \right|}, \qquad (13)$$

where dS is an element of area on a surface of constant δ_k in k space. This allows us to cast all dependence on k into a single factor common to all the integrals of Equation 12:

$$\mathfrak{T}_{i} = \iint \frac{|k_{i}|^{2}}{|\nabla_{k}|\mathcal{E}_{k}|} dS$$
(14)

Here the integrals extend over a surface of constant \mathcal{E}_k . These integrals are evaluated most conveniently in a coordinate system in which the surfaces of constant energy are spherical. Denote the new coordinates by w; then such surfaces must have the form

$$\xi_k = -\xi_w = -\frac{\hbar^2}{2} \left(w_1^{\ 2} + w_2^{\ 2} + w_3^{\ 2} \right) = -\frac{\hbar^2}{2} \ w^2 \ .$$

Comparison with Equation 1 shows that

$$w_i = \frac{k_i}{m_i^{1/2}}$$
.

Thus

$$\begin{split} \mathrm{d}^3 \mathrm{k} & = \left(\, \mathrm{m_1 \, m_2 \, m_3} \right)^{1/2} \, \mathrm{d}^3 \mathrm{w} \\ & = \frac{\triangle^{1/2} \, \mathrm{d} S \, \mathrm{d} \mathcal{E}_{\mathrm{w}}}{\left| \, \bigvee_{\mathrm{w}} \, \mathcal{E}_{\mathrm{w}} \, \right|} = \frac{\triangle^{1/2} \, \mathrm{d} S \, \mathrm{d} \mathcal{E}_{\mathrm{w}}}{| \, \mathrm{h}^2 \, \mathrm{w}} \; . \end{split}$$

But

$$dS = w^2 d/ d(\cos \alpha)$$
,

where and are the polar angles corresponding to w. Therefore

$$\mathfrak{J}_{i} = \int_{-1}^{1} \int_{0}^{2\pi} \frac{\Delta^{1/2} \, m_{i} \, w_{i}^{2} \, w \, d / \, d \langle \cos w \rangle}{\hbar^{5}}$$

$$= \frac{1}{\hbar^{5}} \frac{8}{3} \sqrt{2} \, \pi \, m_{i} \, \Delta^{1/2} \, \xi_{k}^{3/2} .$$
(15)

With these simplifications Equation 12 becomes

$$\mathbf{J} = -\frac{2\sqrt{2} e^{2}}{3\pi^{2} h^{3}} \Delta^{1/2} \left(\int_{0}^{\infty} + \mathcal{E}_{k}^{3/2} \frac{\partial f_{0}}{\partial \mathcal{E}_{k}} d\mathcal{E}_{k} \right) m^{-1} + \mathbf{E}$$

$$+ \frac{2\sqrt{2} e^{3}}{3\pi^{2} h^{3} c} \frac{1}{\Delta^{1/2}} \left(\int_{0}^{\infty} \tau^{2} \mathcal{E}_{k}^{3/2} \frac{\partial f_{0}}{\partial \mathcal{E}_{k}} d\mathcal{E}_{k} \right) (m \cdot \mathbf{H}) + \mathbf{E}$$

$$- \frac{2\sqrt{2} e^{4}}{3\pi^{2} h^{3} c^{2}} \frac{1}{\Delta^{1/2}} \left(\int_{0}^{\infty} \tau^{2} \mathcal{E}_{k}^{3/2} \frac{\partial f_{0}}{\partial \mathcal{E}_{k}} d\mathcal{E}_{k} \right) [\mathbf{H} \mathbf{H} + \mathbf{m}^{-1} + \mathbf{H} + \mathbf{m} + \mathbf{H} +] + \mathbf{E} . \tag{16}$$

The following abbreviations are useful:

$$\mathfrak{N} = \frac{2\sqrt{2} e^2}{3\pi^2 h^3} \wedge^{1/2} .$$

$$\mathfrak{J}^{(n)} = \mathfrak{J} \int_0^{\infty} e^{n} \, \xi_k^{3/2} \, \frac{\partial f_0}{\partial \xi_k} \, d\xi_k . \tag{17}$$

In this notation

$$J = \#^{(1)} \, \mathsf{m}^{-1} + E + \frac{e}{c} \, \frac{1}{\Delta} \#^{(2)} \, \langle \mathsf{m} + \mathsf{H} \rangle \rightarrow E$$

$$-\frac{e^{2}}{c^{2}}\frac{1}{\Delta} \, f^{(3)} \left[H \, H \, \text{-m}^{-1} \, \cdot \, (H \, \cdot \, \text{m} \, \cdot \, H) \, 1 \, \right] \, \cdot \, E \ , \tag{18}$$

the explicit form of the conductivity tensor for a single valley in a weak magnetic field.

Case 2-Strong Magnetic Fields

Substitution of Equation 9 into Equation 10 yields

$$\mathbf{J} = -\frac{\mathrm{e}^{2}}{4\pi^{3}} \int \frac{\tau \, \mathbf{v}_{k} \, \mathbf{v}_{k} + \mathbf{E}}{\mathbf{D}(\mathbf{H})} \, \frac{\partial \, \mathbf{f}_{0}}{\partial \, \mathcal{E}_{k}} \, d^{3}\mathbf{k}$$

$$+ \frac{\mathrm{e}^{2}}{4\pi^{3}} \, \frac{\mathrm{e}}{\mathrm{c}} \int \frac{\tau^{2} \, \mathbf{v}_{k} \, \mathbf{v}_{k} + \mathbf{H} \times \mathbf{m}^{-1} + \mathbf{E}}{\mathbf{D}(\mathbf{H})} \, \frac{\partial \, \mathbf{f}_{0}}{\partial \, \mathcal{E}_{k}} \, d^{3}\mathbf{k}$$

$$- \frac{\mathrm{e}^{2}}{4\pi^{3}} \left(\frac{\mathrm{e}}{\mathrm{c}} \right)^{2} \, \frac{1}{\Delta} \int \frac{\tau^{3} \, \mathbf{v}_{k} \, \mathbf{v}_{k} + \mathbf{m} + \mathbf{H} \, \langle \mathbf{H} + \mathbf{E} \rangle}{\mathbf{D}(\mathbf{H})} \, \frac{\partial \, \mathbf{f}_{0}}{\partial \, \mathcal{E}_{k}} \, d^{3}\mathbf{k} \, , \tag{19}$$

where

$$\mathbf{D}(\mathbf{H}) = -1 + \left(\frac{\tau \mathbf{e}}{\mathbf{c}}\right)^2 \frac{1}{\Delta} \left(\mathbf{H} \cdot \mathbf{m} \cdot \mathbf{H}\right) . \tag{20}$$

All the arguments used in simplifying Equation 12 are also valid in the strong field case, the simplified form of Equation 19 being

$$J = - k^{(1)} (H) m^{-1} \cdot E + \frac{e}{c} \frac{1}{\Lambda} k^{(2)} (H) (m \cdot H) \times E$$

$$- \left(\frac{e}{c}\right)^{2} \frac{1}{\Lambda} k^{(3)} (H) H(H \cdot E) , \qquad (21)$$

where

$$K^{(n)}(\mathbf{H}) = \Re \int_{0}^{\infty} \frac{\tau^{n} \mathcal{E}_{\mathbf{k}}^{3/2}}{\mathbf{D}(\mathbf{H})} \frac{\partial f_{0}}{\partial \mathcal{E}_{\mathbf{k}}} d\mathcal{E}_{\mathbf{k}} . \tag{22}$$

This form differs notably from Equation 18 only in the last term, where all the orientation dependence is contained in the integral $K^{(3)}(H)$.

EXTENSION OF THE THEORY TO MANY VALLEYS

Theory for a Single Crystal

In discussing the model it was observed that, for a model based on anisotropy in the energy band minima to exhibit the symmetry of a real crystal, there must be several such minima distributed according to that symmetry. The properties of the crystal itself will be sums of the properties of differently oriented valleys. This section will discuss the techniques of transforming the results for a minimum of standard orientation into those for minima oriented in other arbitrary directions.

Equations 18 and 21 can be written in the abbreviated form

$$\mathbf{J} = \mathbf{\sigma}(\mathbf{H}) + \mathbf{E} , \qquad (23)$$

where the components of the second rank tensor $\sigma(H)$ may depend on H. The elements of $\sigma(H)$ may be determined from Equations 18 and 21 by inspection. Equation 23 shows that the problem of finding the relation between J and E for various orientations of a valley reduces to the problem of finding how $\sigma(H)$ changes under a rotation of the coordinate system. Thus, if there are N equivalent valleys in the Brillouin zone symmetrically disposed about an axis, the conductivity for a single crystal will be

$$\sigma(\mathbf{H}) = \sum_{i=1}^{N} \sigma^{(i)}(\mathbf{H}) . \tag{24}$$

The tensors $\sigma^{(1)}(H)$ all transform into one another when the coordinate system is rotated through a multiple of $2\pi/N$ radians about the axis of symmetry. The treatment is analogous for other types of symmetry.

If $\sigma(H)$ were a true tensor, a $\sigma'(H)$ could be found in some rotated system merely by applying the transformation A defined by

$$\mathbf{x}' = \mathbf{A} \cdot \mathbf{x} , \qquad (25)$$

where \mathbf{x}' and \mathbf{x} are vectors in the transformed and untransformed spaces, respectively.* For the corresponding second rank tensor transformation, in matrix notation,

$$\sigma = A + \sigma + A^{-1} \tag{26}$$

If, however, $\sigma(H)$ is inserted into Equation 26, a new tensor is found in which the magnetic field H has been rotated with the coordinate system. Consequently, Equation 26 does not preserve the angle between E and H and requires modification. Actually all that is necessary is the application of an inverse transformation to H in the transformed tensor. Thus,

$$\sigma'(\mathbf{H}) = A \cdot \left[\sigma(\mathbf{A}^{-1} \cdot \mathbf{H})\right] \cdot \mathbf{A}^{-1}$$
 (27)

is the correct expression.

In the case of weak magnetic fields the elements of $\sigma(H)$ depend on H in a simple way, and it is possible to streamline the treatment. For strong magnetic fields, however, the dependence of the integrals $h^{(n)}(H)$ on H defies simplification. Both cases will now be treated in detail.

^{*}See any textbook on mechanics, Reference 10 for example.

Case 1-Weak Magnetic Fields

Equation 18 shows that, for weak magnetic fields, $\sigma(H)$ may be expressed as the sum of three tensors:

$$\mathbf{J}_{i} = \sum_{j} \frac{(I)}{ij} \mathbf{E}_{j} + \sum_{jk} \frac{(II)}{ijk} \mathbf{H}_{j} \mathbf{E}_{k} + \sum_{jkl} \frac{(III)}{ijkl} \mathbf{H}_{j} \mathbf{H}_{k} \mathbf{E}_{l} .$$
 (28)

Notice that in this form the v's have no dependence on H. This makes it possible to treat them in the simplified manner of Equation 26 rather than that of Equation 27. Since only one of the tensors is of second rank, matrix notation is no longer convenient. In tensor notation Equation 26 becomes

$$\sigma_{ij}' = \sum_{kl} \mathbf{A}_{ik} \mathbf{A}_{jl} \sigma_{kl}$$
 (29)

Similar expressions hold for σ_{ijk} and σ_{ijk} . From Equation 18,

$$\sigma_{ij}^{(1)} = -\beta^{(1)} \left(m^{-1} \right)_{ij}$$
, (30)

$$\simeq_{ijk}^{(tt)} \qquad \sum_{l} \frac{e}{c} \, \, \mathfrak{g}^{(2)} \, \, \frac{1}{\Delta} \, \, \delta_{i\,lk} \, \, (\mathsf{m})_{\,lj} \, \, , \tag{31}$$

$$= \left(\frac{\text{(III)}}{\text{ijk}^{\perp}}\right) = -\left(\frac{e}{c}\right)^2 \#^{(3)} = \frac{1}{\triangle} \Omega_{\text{ijk}^{\perp}}, \qquad (32)$$

where δ_{iik} is the permutation symbol defined by

0 (any two subscripts equal),

 δ_{ijk} (any even permutation of subscripts),

1 (any odd permutation of subscripts).

The fourth rank tensor Ω_{ijkl} will be discussed after some refinements in notation have been introduced. Applying Equation 29 to Equations 30 and 31 shows

$$\sigma_{i_{j}}^{(\mathbf{I})'} = g^{(\mathbf{I})} \sum_{\mathbf{k}_{i}} \mathbf{A}_{i\mathbf{k}} \mathbf{A}_{j_{i}} \left(\mathbf{m}^{-1} \right)_{\mathbf{k}_{i}}, \tag{33}$$

$$\sigma_{ijk}^{(II)'} = \frac{e}{c} \frac{1}{\Delta} \beta^{(2)} \sum_{lmn} \mathbf{A}_{il} \mathbf{A}_{jm} \mathbf{A}_{kn} \delta_{lpn} \langle \mathbf{m} \rangle_{pm} . \tag{34}$$

Since $A_{ik} = (A^{-1})_{ki}$, the first of these may be written in matrix notation as

$$\sigma^{(1)}' = - \mathfrak{g}^{(1)} A \cdot m^{-1} \cdot A^{-1}$$

$$= - \mathfrak{g}^{(1)} (\mathfrak{m}^{-1})' . \tag{35}$$

The second becomes

$$\sigma_{ijk}^{(II)'} = \frac{e}{c} \frac{1}{\Delta} \mathfrak{g}^{(2)} \sum_{lmn} \mathbf{A}_{il} \delta_{lpn}^{(m)} (\mathbf{m})_{pm} (\mathbf{A}^{-1})_{mj} (\mathbf{A}^{-1})_{nk} . \tag{36}$$

If we multiply this into H₁ and contract, we can write in matrix language,

$$\sigma^{(II)'}(H) = \frac{e}{c} \frac{1}{\Delta} \mathfrak{g}^{(2)} A \cdot \left[\left(m \cdot A^{-1} \cdot H \right) \times \right] \cdot A^{-1}$$

$$= A \cdot \left[\sigma^{(II)} \left(A^{-1} \cdot H\right)\right] \cdot A^{-1} , \qquad (37)$$

in agreement with Equation 27.

To write down an expression for Ω_{ijkl} in Equation 32, consider it a transformation of the *dyadic* HH rather than of the vector $\mathbf{H}(\mathbf{H} \cdot \mathbf{E})$. Since HH is a symmetric tensor, the notation of elasticity theory* may be used to write it as a six-dimensional vector:

$$HH \longrightarrow (H_1 H_1, H_2 H_2, H_3 H_3, H_2 H_3, H_3 H_1, H_1 H_2) . \tag{38}$$

Then Ω_{iikl} may be written as a square six-dimensional matrix:

$$\Omega = \left(- \left(\mathbf{m}^{-1} \right) \left(\mathbf{m} \right) \right) , \tag{39}$$

where I is the six-dimensional unit matrix and (m^{-1}) (m) is not a matrix product but a dyadic formed from 2 six-dimensional vectors (three components of which vanish, since m and m^{-1} are diagonal in

^{*}See any discussion of elasticity theory, for example Reference 11 or 12.

this coordinate system). Thus

$$\Omega = \begin{bmatrix} 0 & -\frac{m_2}{m_1} & -\frac{m_3}{m_1} & 0 & 0 & 0 \\ -\frac{m_1}{m_2} & 0 & -\frac{m_3}{m_2} & 0 & 0 & 0 \\ -\frac{m_1}{m_3} & -\frac{m_2}{m_3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$(40)$$

Evidently Ω is not symmetric. Although this notation makes it possible to write the fourth rank tensor in matrix form, it is not particularly useful for calculations. The transformation of a fourth rank tensor is analogous to Equation 29:

$$\Omega'_{imip} = \sum_{hijk} \mathbf{A}_{in} \mathbf{A}_{mi} \mathbf{A}_{nj} \mathbf{A}_{pk} \Omega_{hijk} . \tag{41}$$

Hearmon gives a table of these coefficients for the case of a *symmetric* fourth rank tensor (Reference 13). A similar table for the nonsymmetric case would be much longer but would contain no new combinations. In any case, it is not difficult to deduce such a table from Equation 41.

With the help of Equations 33, 34, and 41 expressions for $\phi_{ij}^{(II)}$, $\phi_{ijk}^{(III)}$, and $\phi_{ijk}^{(III)}$ in Equation 28 may be found which are valid for any orientation of the coordinate system. The particular form of the transformation matrix A is arbitrary, but one alternative is:

Figure 1 depicts the choice of angles (the Euler angles) for this form.

It is still necessary to find the particular transformations which carry the standard valley into all the others, perform the transformations, and sum to find the total conductivity. These computations rely on the particular symmetry of the crystal and will not be performed here. It should be mentioned that in many cases more than one distribution of valleys may satisfy the symmetry requirements. Drabble and Wolfe give a treatment similar to the one here, but modified to show explicitly the separate roles of crystal symmetry and choice of distribution (Reference 14). The present treatment, however, is more appropriate for the averaging process to be discussed later.

Table 1 lists references in which explicit calculations have been carried out for particular models and particular crystal symmetries. In cases for which the computations have not been performed, simply determine A and follow the procedure outlined here or that in Reference 14.

Case 2-Strong Magnetic Fields

In analogy with Equation 28, Equation 21 may be rewritten:

$$J_{i} = \sum_{j} [\sigma^{(I)}(H)]_{ij} E_{j} + \sum_{jk} [\sigma^{(II)}(H)]_{ijk} H_{j} E_{k} + \sum_{jkl} [\sigma^{(III)}(H)]_{ijkl} H_{j} H_{k} E_{l} , \qquad (43)$$

where

$$\left[\sigma^{(1)}(\mathbf{H})\right]_{ij} = -K^{(1)}(\mathbf{H})\left(\mathbf{m}^{-1}\right)_{ij},$$
 (44)

$$\left[\sigma^{(II)}(\mathbf{H})\right]_{ijk} = \sum_{i} \frac{e}{c} \frac{1}{\Delta} K^{(2)}(\mathbf{H}) \delta_{ilk} (\mathbf{m})_{lj}, \qquad (45)$$

$$\left[\sigma^{(III)}(\mathbf{H})\right]_{ijkl} = -\left(\frac{e}{c}\right)^2 \frac{1}{\Delta} K^{(3)}(\mathbf{H}) \delta_{ij}\delta_{kl}. \tag{46}$$

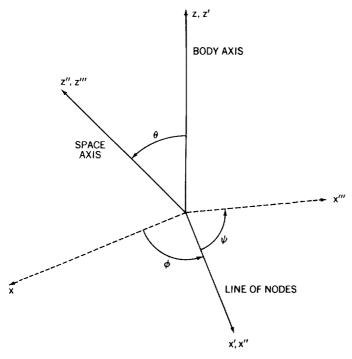


Figure 1—Definition of the Euler angles ϕ , θ , and ψ .

Table 1

References for Explicit Calculations of Magnetoconductivity Coefficients for Single Crystals.

Crystal Symmetry	Model	Refer- ences
Cubic	6 ellipsoids, $m_1 = m_2 \neq m_3$	3, 4
(m3m)	12 ellipsoids, $m_1 = m_2 \neq m_3$	4
	8 ellipsoids, $m_1 = m_2 \neq m_3$	3, 4
Trigonal	1 ellipsoid, $m_1 = m_2 \neq m_3$	15
(3 m)	3 ellipsoids, $m_1 \neq m_2 \neq m_3$	15
	6 ellipsoids, $m_1 \neq m_2 \neq m_3$	14

Notice that the complicated fourth rank tensor \cup_{ijkl} of the weak field case has been replaced by the form δ_{ij} δ_{kl} . This transforms quite simply:

$$\left(\delta_{h_{1}} \delta_{jk} \right)' = \sum_{l m n p} \mathbf{A}_{h_{l}} \mathbf{A}_{im} \mathbf{A}_{jn} \mathbf{A}_{kp} \delta_{lm} \delta_{np}$$

$$\sum_{l n} \mathbf{A}_{h_{l}} \left(\mathbf{A}^{-1} \right)_{l,i} \mathbf{A}_{jn} \left(\mathbf{A}^{-1} \right)_{nk}$$

$$\delta_{h,i} \delta_{jk} = 0$$

$$(47)$$

Transforming any of the tensors in Equation 44-46 yields Equation 33, 34, or 47 multiplied by a factor containing

$$\mathcal{H}^{(n)}\left(\mathbf{A}^{-1} \cdot \mathbf{H}\right) = \mathcal{H} \int_{0}^{\infty} \frac{\tau^{n} \mathcal{E}_{k}^{3/2} \frac{\partial f_{0}}{\partial \mathcal{E}_{k}}}{1 + \omega \left[\left(\mathbf{A}^{-1} \cdot \mathbf{H}\right) + \mathbf{m} + \left(\mathbf{A}^{-1} \cdot \mathbf{H}\right)\right]} d\mathcal{E}_{k} , \qquad (48)$$

where

$$L = \frac{1}{\Delta} \left(\frac{\tau e}{c} \right)^2 .$$

Notice that

$$\begin{array}{lll} \left({{{\bf{A}}^{ - 1}} \cdot {\bf{H}}} \right) + {{\bf{m}}} \cdot \left({{{\bf{A}}^{ - 1}} \cdot {\bf{H}}} \right) & & \sum\limits_{i j k l} {{\left({{{\bf{A}}^{ - 1}}} \right)}_{i j}} \; {{\bf{H}}_j} \; {{\bf{I}}_m} \right)_{i k}} \; {{\left({{{\bf{A}}^{ - 1}}} \right)}_{k l}} \; {{\bf{H}}_l} \\ \\ & \sum\limits_{i j k l} {{{\bf{H}}_j} \; {{\bf{A}}_j}_{i k}} \; {{\left({{{\bf{A}}^{ - 1}}} \right)}_{k k}} \; {{\left({{{\bf{A}}^{ - 1}}} \right)}_{k l}} \; {{\bf{H}}_l}} \\ \\ & {{\bf{H}} \cdot \left({{\bf{A}} \cdot {\bf{m}} \cdot {\bf{A}}^{ - 1}} \right) + {\bf{H}}} \\ \\ & {{\bf{H}} \cdot {\bf{m}}' + {\bf{H}}} \; . \end{array}$$

as might have been expected. In actual calculations the integrals of Equation 48 must be evaluated with a computer. The integrals for different ellipsoids will differ only in the constant term in the denominator. Aside from this complication, the procedure used here is exactly analogous to that used for the case of weak magnetic fields.

Theory for Polycrystalline Materials

As the name implies, a polycrystalline material consists of a large number of distinct single crystals. This section is a discussion of properties of such materials when the individual crystals are *randomly oriented*. Without this assumption the theory is prohibitively complex.

If the crystals are randomly oriented, the material will not exhibit direction-dependent properties. In this case the material is said to be *quasi isotropic* because, even though the constituent crystals may be anisotropic, a large sample possesses isotropic symmetry. The procedure adopted here for calculating the tensor properties of a quasi isotropic substance has been described by Voight for elastic properties (Reference 11). Keyes has applied this procedure to the conductivities in the presence of a weak magnetic field (Reference 16). His results will be derived for case 1 and the treatment extended to the strong field, case 2.

The total current flowing through an imaginary plane of area S in the material must be the sum of the contributions from each of the crystals cut by the plane. If the area of the i^{th} "sliced" crystal is s_i , then the total current through the plane is

$$I = \sum_{i} s_{i} \cdot \sigma_{i} \cdot E_{i} , \qquad (49)$$

where $|\mathbf{s}_i| = \mathbf{s}_i$. The vector $\mathbf{s}_i/|\mathbf{s}_i|$ is normal to the area element \mathbf{s}_i . \mathbf{E}_i and σ_i both refer to the i^{th} crystal. From this expression it can be seen that the size of the crystals must not be correlated with their orientation. Obviously, if crystals with a special orientation tend to be larger than average, their properties will dominate those of the entire material, spoiling the isotropic symmetry.

One further assumption is required for a manageable theory. Since Equation 49 gives no information about E_i , it must be assumed to remain constant over the entire plane S. This is simpler than the alternative assumption that J is constant over the cross section. In that case the conductivity tensor for the crystal would have to be inverted and the resulting resistivity tensor summed. But this requires detailed knowledge of the crystal symmetry and valley distribution. To sum the conductivity tensor, we need only add the contributions of all the valleys throughout the material, which, for random orientation, amounts to multiplying the orientation average of a single valley by the number of valleys. Certainly neither of these assertions is entirely realistic, and the alternative which agrees best with experiment must be chosen. Keyes has discussed this problem and found that the two alternatives do not give widely divergent results (Reference 16). Indeed, when the constituent crystals have cubic symmetry the results are identical.

Thus Equation 49 may be rewritten as

$$I = S \cdot \left(\sum_{i} \sigma_{i}\right) \cdot E ,$$

where, for a large number of crystals,

$$\sum_{i} \sigma_{i} \rightarrow \frac{N}{8\pi^{2}} \int_{0}^{2\pi} \int_{-1}^{1} \int_{0}^{2\pi} \sigma(\phi, \psi) d\phi d(\cos \psi) d\psi , \qquad (50)$$

for random orientation of the individual crystals. N is the total number of valleys. Here advantage is taken of the fact that the conductivity tensor for an arbitrary choice of a coordinate system is a function of the elements of the rotation matrix A, which are in turn functions of the angles specifying the rotation. In that which follows Equation 50 will be applied systematically to each of the expressions for $\sigma(H)$ derived previously.

Case 1-Weak Magnetic Fields

In this case Equation 50 is applied directly to each of the tensors defined in Equation 28. The computation is reduced considerably by taking advantage of the known symmetry of the quasi isotropic material. In such a material the conductivity is a scalar and the Hall conductivity is proportional to $\mathbf{H} \times \mathbf{E}$. Thus $\langle \sigma^{(1)} \rangle$ has the form $\sigma^{(1)} \otimes_{ij} (\text{where } \sigma^{(1)})$ is a scalar) and is completely determined by the orientation average of a single diagonal element of $\sigma^{(1)}$. From Equations 33 and 50

$$\left[\left[\sigma^{(1)} \right]_{33} \right] = -\frac{4}{3} (1) \frac{N}{8\pi^2} \int_0^{2\pi} \int_{-1}^1 \int_0^{2\pi} \sum_{kl} A_{3k} A_{3l} \left(m^{-1} \right)_{kl} d\phi d(\cos \theta) d\phi$$

$$= -\frac{4}{3} (1) \frac{N}{8\pi^2} \int_0^{2\pi} \int_{-1}^1 \int_0^{2\pi} \left(\frac{1}{m_1} \sin^2 \theta \sin^2 \psi + \frac{1}{m_2} \sin^2 \theta \cos^2 \psi + \frac{1}{m_3} \cos^2 \theta \right) d\phi d(\cos \theta) d\psi$$

$$= -\frac{4}{3} (1) N \frac{1}{3} \left(\frac{1}{m_1} + \frac{1}{m_2} + \frac{1}{m_3} \right)$$

$$= -\frac{4}{3} (1) N \frac{1}{3} \left(\frac{1}{m_1} + \frac{1}{m_2} + \frac{1}{m_3} \right)$$
(51)

An entirely similar argument leads to:

$$\sigma(II) = \frac{e}{c} \mathfrak{g}(2) N \frac{1}{3} \left(\frac{1}{m_2 m_3} + \frac{1}{m_3 m_1} + \frac{1}{m_1 m_2} \right) . \tag{52}$$

The average for Ω_{ijkl} is found in precisely the same manner: Insert the expressions for the elements of the transformation matrix into Equation 41 and average over all orientations. Voight (Reference 11) has shown that a fourth rank tensor describing a property of an isotropic material must have

the appearance:

$$\begin{bmatrix} c & c_1 & c_1 & 0 & 0 & 0 \\ c_1 & c & c_1 & 0 & 0 & 0 \\ c_1 & c_1 & c & 0 & 0 & 0 \\ 0 & 0 & 0 & c_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & c_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & c_2 \end{bmatrix}. \tag{53}$$

where $c_2 = \begin{pmatrix} c & c_1 \end{pmatrix}$ in the notation used here. Thus it is only necessary to compute averages for *two* elements. The details will be omitted here: Voight has done the computation for a symmetric fourth rank tensor, and Keyes has obtained a similar result for the nonsymmetric case (Reference 16). In the notation used here the appropriate averages are

$$\frac{1}{15} \left(\frac{m_2 + m_3}{m_1} + \frac{m_3 + m_1}{m_2} + \frac{m_1 + m_2}{m_3} \right) + \frac{2}{5} ,$$

$$\frac{2}{15} \left(\frac{m_2 + m_3}{m_1} + \frac{m_3 + m_1}{m_2} + \frac{m_1 + m_2}{m_3} \right) - \frac{1}{5} .$$

$$\frac{1}{15} \left(\frac{m_2 + m_3}{m_1} + \frac{m_3 + m_1}{m_2} + \frac{m_1 + m_2}{m_3} \right) + \frac{3}{5} .$$
(54)

Keyes defines an anisotropy parameter

$$\Lambda = \frac{1}{2} \left(\frac{m_2 + m_3}{m_1} + \frac{m_3 + m_1}{m_2} + \frac{m_1 + m_2}{m_3} \right) - 3$$

$$= \frac{1}{2} \frac{1}{\Delta} \left[m_1 \left(m_3 - m_2 \right)^2 + m_2 \left(m_1 - m_3 \right)^2 + m_3 \left(m_2 - m_1 \right)^2 \right] . \tag{55}$$

in terms of which

Equations 51, 52, and 56 provide the averages which, substituted into Equation 28, give the conductivity, Hall conductivity, and magnetoconductivity appropriate for the quasi isotropic case. Thus

$$\left\langle \sigma^{(11)} \right\rangle_{ijk} = -\frac{4}{3} \left(\frac{1}{3} \left(\frac{1}{m_{1}} + \frac{1}{m_{2}} + \frac{1}{m_{3}} \right) \delta_{ij} \right),$$

$$\left\langle \sigma^{(11)} \right\rangle_{ijk} = -\frac{e}{c} \left(\frac{1}{2} \right) N \frac{1}{3} \left(\frac{1}{m_{2} m_{3}} + \frac{1}{m_{3} m_{1}} + \frac{1}{m_{1} m_{2}} \right) \delta_{ijk} \right)$$

$$\left\langle \sigma^{(111)} \right\rangle_{ijk} = -\left(\frac{e}{c} \right)^{2} \left(\frac{1}{3} \right) N \frac{1}{\Delta} \left\langle \Omega_{ijk} \right| \right\rangle.$$
(57)

Case 2-Strong Magnetic Fields

Equations 44-46 show that for a quasi isotropic material in a strong magnetic field the three conductivity tensors are all scalars multiplied by one of the tensors δ_{ij} , δ_{ijk} , or $\delta_{ij}\delta_{kl}$. Thus only one integration per tensor is necessary to fix the entire average expression. Accordingly, the averages of $\left[\sigma^{(1)}(H)\right]_{33}$, $\left[\sigma^{(11)}(H)\right]_{123}$, and $\left[\sigma^{(111)}(H)\right]_{1111}$ will be computed. First, however, it is necessary to make two assumptions that simplify the computations considerably: Let the magnetic field point along the positive z direction, $H=\left(0,0,H_3\right)$, and let the energy surfaces be ellipsoids of revolution, $m_1=m_2$. The latter assumption is no more than an artifice to ease the labor of computation, but nevertheless it imposes a restriction on the generality of our model. It is not a serious limitation, since in actual practice masses other than the transverse $\left(m_1\right)$ and longitudinal $\left(m_3\right)$ are rarely used to characterize an anisotropic energy surface. Moreover, the symmetry of the crystal under consideration requires that $m_1=m_2$ if the z axis is one of rotational symmetry.

With this understood, we may write

$$\left\langle \left[\sigma^{(1)} (\mathbf{H}) \right]_{33} \right\rangle = -\frac{N}{8\pi^2} \int_0^1 \int_0^1 \int_0^{2\pi} \int_0^{\infty} \frac{\Re \varepsilon_k^{3/2} \frac{\partial f_0}{\partial \xi_k}}{1 + e(\mathbf{H} \cdot \mathbf{m} \cdot \mathbf{H})} \left(\frac{1}{m_1} \sin^2 \theta + \frac{1}{m_3} \cos^2 \theta \right) d\xi_k d\phi d(\cos \theta) d\psi, \tag{58}$$

where

$$\mathbf{H} + \mathbf{m}' + \mathbf{H} = \mathbf{H}_3^2 \left(\mathbf{m}_1 \sin^2 \theta + \mathbf{m}_3 \cos^2 \theta \right) . \tag{59}$$

With the substitution

$$N \Re \tau^{n} \, \mathcal{E}_{k}^{3/2} \, \frac{\partial f_{0}}{\partial \mathcal{E}_{k}} = F^{(n)} \left(\mathcal{E}_{k} \right) . \tag{60}$$

Equation 58 may be rewritten as

$$\left[\left[\sigma^{(1)}(\mathbf{H}) \right]_{33} \right) = -\frac{1}{2} \int_{0}^{1} \int_{0}^{\infty} \frac{F^{(1)}\left(\mathcal{E}_{k}\right) \frac{1}{m_{1}} \left[1 - \frac{1}{m_{3}} \left(m_{3} - m_{1} \right) | \mathbf{x}^{2} \right]}{1 + \omega H_{3}^{2} \left[m_{1} + \left(m_{3} - m_{1} \right) | \mathbf{x}^{2} \right]} d\mathcal{E}_{k} d\mathbf{x}$$

$$= -\int_{0}^{\infty} \frac{F^{(1)}\left(\mathcal{E}_{k}\right) \frac{1}{m_{1}}}{\omega H_{3}^{2} \left| m_{3} - m_{1} \right|} \frac{1}{a} \frac{\tan^{-1}\left(\frac{1}{a}\right) d\mathcal{E}_{k}}{\tan^{-1}\left(\frac{1}{a}\right) d\mathcal{E}_{k}}$$

$$-\int_{0}^{\infty} \frac{F^{(1)}\left(\mathcal{E}_{k}\right) \frac{1}{m_{1}m_{3}} \left| m_{3} - m_{1} \right| a}{\omega H_{3}^{2} \left| m_{3} - m_{1} \right|} \frac{\tan^{-1}\left(\frac{1}{a}\right) d\mathcal{E}_{k}}{\tan^{-1}\left(\frac{1}{a}\right) d\mathcal{E}_{k}} \xrightarrow{m_{3}^{2} \leq m_{1}^{2}}, \tag{61}$$

where

$$a = \sqrt{\frac{1 + \omega H_3^2 m_1}{\omega H_3^2 |m_3 - m_1|}}$$

and $x = \cos \theta$. The functions $\tan^{-1} (1/a)$ and $\tan^{-1} (1/a)$ are to be used for the cases $m_3 > m_1$ and $m_3 < m_1$, respectively. Evidently when $m_1 = m_3$ this reduction is not possible. Then, however, all the angular integrations in Equation 58 are trivial, and an energy integral remains which must be computed numerically in any case. Equation 61 may be rewritten as

$$\left\langle \left[\sigma^{(1)}(\mathbf{H}) \right]_{33} \right\rangle = - \int_{0}^{\infty} \frac{F^{(1)}\left(\mathcal{E}_{k}\right) \frac{1}{m_{1}} a}{1 + \omega H_{3}^{2} m_{1}} \left(1 + \frac{1 + m_{1}\omega H_{3}^{2}}{m_{3}\omega H_{3}^{2}} \right) \frac{\tan^{-1}\left(\frac{1}{a}\right) d\mathcal{E}_{k}}{\tanh^{-1}\left(\frac{1}{a}\right) d\mathcal{E}_{k}} \xrightarrow{m_{3} < m_{1}} . \tag{62}$$

Next compute

$$\left< \left[\sigma^{(11)} \left(H \right) \right]_{123} \right> \; = \; \frac{e}{c} \, \frac{1}{\Delta} \, \frac{1}{8\pi^2} \! \int_0^{2\pi} \! \int_0^1 \int_0^{2\pi} \! \int_0^{\infty} \frac{F^{(2)} \left(\xi_k \right) \! \left[m_1 \left(\sin^2 \! \psi \! + \! x^2 \cos^2 \! \psi \right) \! + \! m_3 \left(1 - \! x^2 \right) \cos^2 \! \psi \right]}{1 + \omega \, H_3^{\; 2} \left[m_1 + \left(m_3 - m_1 \right) \, x^2 \right]} \, d\xi_k \, d\psi \, dx \, d\phi \; .$$

Performing the ϕ and ψ integrations results in

$$\left\langle \left[\ \sigma^{(11)} \left(H \right) \right]_{123} \right\rangle \ = \ \frac{e}{c} \, \frac{1}{\Delta} \, \frac{1}{2} \, \int_{-1}^{1} \, \int_{0}^{\infty} \, \frac{\frac{1}{2} \, \, F^{(2)} \! \left(\mathcal{E}_{k} \right) \left[\left(m_{1} + m_{3} \right) - \left(m_{3} - m_{1} \right) \, x^{2} \right]}{1 \, + \, \omega H_{3}^{\, 2} \left[m_{1} \, + \left(m_{3} - m_{1} \right) \, x^{2} \right]} \, \, d\mathcal{E}_{k} \, \, dx \quad ,$$

which is similar to the form for $\langle \sigma^{(1)}(H) \rangle$. Thus,

$$\left\langle \left[\sigma^{(II)}(\mathbf{H}) \right]_{123} \right\rangle = \frac{1}{2} \frac{e}{c} \frac{1}{\Delta} \int_{0}^{\infty} \frac{\mathbf{F}^{(2)}(\xi_{k}) \mathbf{a}}{1 + \omega \mathbf{H}_{3}^{2} \mathbf{m}_{1}} \left[\left(\mathbf{m}_{1} + \mathbf{m}_{3} \right) + \frac{1 + \omega \mathbf{H}_{3}^{2} \mathbf{m}_{1}}{\omega \mathbf{H}_{3}^{2}} \right] \frac{\tan^{-1}(1 + \omega \mathbf{H}_{3}^{2} \mathbf{m}_{1})}{\tan^{-1}(1 + \omega \mathbf{H}_{3}^{2} \mathbf{m}_{1})} d\xi_{k} + \frac{\mathbf{m}_{3} + \mathbf{m}_{1}}{\mathbf{m}_{3} + \mathbf{m}_{1}} . \tag{63}$$

Finally,

$$\left\langle \left[\sigma^{(\text{III})}(\mathbf{H}) \right]_{1111} \right\rangle = -\left(\frac{e}{c} \right)^{2} \frac{1}{\Delta} \frac{1}{8\pi^{2}} \int_{0}^{2\pi} \int_{-1}^{1} \int_{0}^{2\pi} \int_{0}^{\infty} \frac{\mathbf{F}^{(3)}(\xi_{k})}{1 + \omega H_{3}^{2} \left[m_{1} + \left(m_{3} - m_{1} \right) \mathbf{x}^{2} \right]} d\xi_{k} d\phi d\mathbf{x} d\psi$$

$$= -\left(\frac{e}{c} \right)^{2} \frac{1}{\Delta} \int_{0}^{\infty} \frac{\mathbf{F}^{(3)}(\xi_{k}) \mathbf{a}}{1 + \omega H_{3}^{2} m_{1}} \frac{\tan^{-1}(\frac{1}{a}) d\xi_{k}}{\tanh^{-1}(\frac{1}{a}) d\xi_{k}} \frac{m_{3} > m_{1}}{m_{3} < m_{1}} . \tag{64}$$

This expression, together with Equations 62 and 63, gives the form of the strong field conductivity tensor $\langle \sigma(H) \rangle$ for polycrystalline materials:

$$J_{i} = \sum_{j} \left\langle \sigma^{(1)}(\mathbf{H}) \right\rangle \delta_{ij} E_{j} + \sum_{jk} \left\langle \sigma^{(11)}(\mathbf{H}) \right\rangle \delta_{ijk} H_{j} E_{k} + \sum_{jkl} \left\langle \sigma^{(111)}(\mathbf{H}) \right\rangle \delta_{ij} \delta_{kl} H_{j} H_{k} E_{l} . \tag{65}$$

This completes the extension of the strong field theory to polycrystalline materials.

CONCLUSION

This report has described, in as simple and straightforward a manner as possible, how the many valley model of energy band structure gives results for polycrystalline materials. It must be emphasized that these results rely on the assumptions introduced at the beginning of the section on the "Theory for Polycrystalline Materials" and care must be exercised in using them to interpret experimental data. The method has the advantage that it requires no detailed knowledge of energy band structure to obtain information about the anisotropy of the material. That such information can be obtained from polycrystalline samples is a pleasant surprise, since the preparation of single crystals is often a difficult and expensive task.

The energy integrals that arise in the strong field case in the section mentioned above require further investigation. Their strong dependence on the effective mass ratio suggests that strong field measurements on polycrystalline materials may yield valuable information on this parameter.

ANNOTATED BIBLIOGRAPHY

The following articles supplement the discussion given here. Only papers which discuss the galvanomagnetic effects have been included, but references to treatments of other crystal properties may be found in these. Articles in the list of references which are not in this bibliography do not contain extended discussions of the galvanomagnetic effects.

- 1. Wilson, A. H., "The Theory of Metals" (Reference 7). Section 8.51 gives a solution of the isotropic Boltzmann equation for arbitrary magnetic fields, and section 8.55 gives the weak field expansion for anisotropy in a single minimum in the energy band. No assumption is made concerning the shape of the energy band, and the effective mass formalism is not used. The many valley theory had not yet been formulated when this book was written.
- 2. Blatt, F. J., "Theory of Mobility of Electrons in Solids," in: Solid State Physics: Advances in Research and Applications (Reference 8). Section IV of this review discusses nonspherical energy surfaces and anisotropic relaxation times. The treatment follows that of Wilson (Reference 7) and Herring (Reference 5) very closely. A good discussion on solving the anisotropic Boltzmann equation by transformation to a spherically symmetric system is included. The list of references in this article is more extensive than in any other listed here.
- 3. Abeles, B., and Meiboom, S., "Theory of the Galvanomagnetic Effects in Germanium," *Phys. Rev.* vol. 95, pp. 31-37 (Reference 3). This is one of the first papers to appear on the many valley model and is the best treatment of the galvanomagnetic effects. The presentation is rigorous and almost self-contained, but extremely concise. Only here and in Shibuya's paper (Reference 4) is the strong magnetic field case discussed in detail.
- 4. Shibuya, M., "Magnetoresistance Effect in Cubic Semiconductors with Spheroidal Energy Surfaces," *Phys. Rev.* vol. 95, pp. 1385-1393 (Reference 4). This paper appeared independently of the previous article but treats essentially the same problems. Results are given here in somewhat more detail, but the derivations are more abbreviated.
- 5. Herring, C., "Transport Properties of a Many-Valley Semiconductor," *Bell System Tech. J.*, vol. 34, pp. 237-290 (Reference 5). A wealth of topics is discussed here: mobility (and its temperature dependence for intervalley scattering), thermoelectric power, piezoresistance, Hall effect, high frequency dielectric constant, and magnetoresistance. Approximate Maxwell-Boltzmann statistics are employed throughout, and the notation differs considerably from that used here. The results for the magnetoresistance are obscured by a complicated notation which nevertheless is useful for comparisons with observations.
- 6. Herring, C., and Vogt, E. "Transport and Deformation-Potential Theory for Many-Valley Semiconductors with Anisotropic Scattering," *Phys. Rev.* vol. 101, pp. 944-961 (Reference 6). This report includes a discussion of anisotropic relaxation time and extends deformation potential theory of electron-phonon interaction to the anisotropic case.

- 7. Drabble, J. R., and Wolfe, R., "Anisotropic Galvanomagnetic Effects in Semiconductors," *Proc. Phys. Soc. Section B* vol. 69, pp. 1101-1108 (Reference 14). This paper shows the relation between the components of the resistivity tensor and those of the conductivity tensor, and lists the explicit evaluation of the energy integrals in the cases of weak and extreme degeneracy. A distinction between the model for valley distribution and the requirements of crystal symmetry is drawn to allow use of the known group of symmetry transformations in computing the total conductivity for a single crystal.
- 8. Keyes, R. W., "Isotropic Approximation to the Magnetoresistance of a Multivalley Semiconductor," *Phys. Rev.* vol. 109, pp. 43-46 (Reference 16). Keyes gives the averaging procedure for low field conductivity, Hall conductivity, and magnetoconductivity and inverts to find the corresponding resistivities. A brief discussion of the validity of averaging techniques for the resistivity is found here. The present paper follows the notation of this paper closely especially for case 1 in the section on the "Theory for Polycrystalline Materials," where the treatment parallels that of Keyes. (Footnote 4 in Keyes' paper should be "Adv. in Phys. Vol. 5, 323, 1956," instead of "Phil. Mag. Vol. 5, 323, 1956.")

REFERENCES

- 1. "Proceedings of the International Conference on Semiconductor Physics," Czechoslovak Acad. Sci., Prague, 1962.
- 2. Olechna, D. J., and Ehrenreich, H., "Mobility and Thermoelectric Power in Many-Valley Polar Semiconductors J. Phys. Chem. Solids 23:1513-1520, 1962.
- 3. Abeles, B., and Meiboom, S., "Theory of the Galvanomagnetic Effects in Germanium," *Phys. Rev.* 95(1):31-37, July 1, 1954.
- 4. Shibuya, M., "Magnetoresistance Effect in Cubic Semiconductors with Spheroidal Energy Surfaces," *Phys. Rev.* 95(6):1385-1393, September 15, 1954.
- 5. Herring, C., "Transport Properties of a Many-Valley Semiconductor," *Bell Syst. Tech. J.* 34(2): 237-290, March, 1955.
- 6. Herring, C., and Vogt, E., "Transport and Deformation-Potential Theory for Many-Valley Semi-conductors with Anisotropic Scattering," *Phys. Rev.* 101(3):944-961, February 1, 1956.
- 7. Wilson, A. H., "The Theory of Metals," 2nd ed., Cambridge: University Press, 1953.
- 8. Blatt, F. J., "Theory of Mobility of Electrons in Solids," in: *Solid State Physics*, ed. by F. Seitz and D. Turnbull, New York: Academic Press, Inc., 1957, vol. 4, pp. 200-366.
- 9. McClure, J. W., "Field Dependence of Magnetoconductivity," *Phys. Rev.* 101(6):1642-1646, March 15, 1956.
- 10. Goldstein, H., "Classical Mechanics," Reading, Massachusetts: Addison Wesley, 1959.

- 11. Voight, W., "Lehrbuch der Kristallphysik," Leipzig, Teubner, 1928.
- 12. Kittel, C., "Introduction to Solid State Physics," 2nd ed., New York: Wiley, 1956.
- 13. Hearmon, R. F. S., "The Elastic Constants of Anisotropic Materials—II," *Adv. in Phys.* 5(19): 323-382, July 1956.
- 14. Drabble, J. R., and Wolfe, R., "Anisotropic Galvanomagnetic Effects in Semiconductors," *Proc. Phys. Soc.*, Section B. 69(11):1101-1108, November 1956.
- 15. Abeles, B., and Meiboom, S., "Galvanomagnetic Effects in Bismuth," *Phys. Rev.* 101(2):544-550, January 15, 1956.
- 16. Keyes, R. W., "Isotropic Approximation to the Magnetoresistance of a Multivalley Semiconductor," *Phys. Rev.* 109(1):43-46, January 1, 1958.

22 G-423

NASA TN D-1840	Marburger. John H.,
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